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Modeling wax formation with predictive UNIQUAC: from petroleum and fuels to biofuels

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A decade ago a model was proposed by us to describe the wax formation in crude oils and distillate fuels. Based on the Predictive UNIQUAC concept the model was very successful and was widely adopted by the industry [1].

With the advent of biofuels the incorporation of methyl or ethyl esters in the diesel was required and the presence of saturated long chain esters in solution created new problems of using these fuels at low temperatures. Aiming at understanding the low temperature behavior of vegetable oils and biodiesel fuels an extensive study of the binary systems of fatty acids [2], fatty acid methyl esters [3] and fatty acid ethyl esters [4] of even numbered fatty acid alkyl chains was carried.

In this lecture the binary phase diagrams of these mixtures will be presented. It will be shown how, depending on the alkyl chain length differences in the binaries, it is possible to observe systems that change from a simple eutectic mixture to others where partial solid solution, formation of intermediate compounds, eutectic, peritectic and even metatetic reactions are observed. Considering the composition of a biodiesel the relevance of these binary mixtures to the understanding of cloud point formation of biodiesels will be discussed.

Finally it will be shown how the Predictive UNIQUAC model can describe the phase behavior of biodiesel fuels at temperatures below their cloud point with an accurate description of the changes on the liquid phase and solid phase being formed [5]. A discussion concerning the future developments of this research field, in particular the modeling of diesel-biodiesel blends will conclude this presentation.

References

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